

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelxl

Bond precision: Cu- O = 0.0030 A Wavelength=0.71069

Cell: a=7.7119(8) b=10.5245(9) c=7.8034(9)
 alpha=90 beta=103.862(5) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	614.91(11)	614.91(11)
Space group	P 21/c	P1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Cu3 O14 P4, 2(Rb)	Cu3 O14 P4, 2(Rb)
Sum formula	Cu3 O14 P4 Rb2	Cu3 O14 P4 Rb2
Mr	709.47	709.47
Dx,g cm ⁻³	3.832	3.832
Z	2	2
Mu (mm ⁻¹)	13.607	13.607
F000	666.0	666.0
F000'	665.40	
h,k,lmax	10,13,10	10,13,10
Nref	1409	1403
Tmin,Tmax	0.282,0.506	0.340,0.583
Tmin'	0.188	

Correction method= NUMERICAL

Data completeness= 0.996 Theta(max)= 27.500

R(reflections)= 0.0304(1361) wR2(reflections)= 0.0692(1403)

S = 1.136 Npar= 106

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT774_ALERT_1_C	Suspect X-Y Bond in CIF:	RB1	--	O4	..	3.62 Ang.
PLAT774_ALERT_1_C	Suspect X-Y Bond in CIF:	RB1	--	P2	..	3.64 Ang.
PLAT774_ALERT_1_C	Suspect X-Y Bond in CIF:	O4	--	RB1	..	3.62 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance				2.137

PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min)	5
PLAT975_ALERT_2_C Positive Residual Density at 0.90A from O2	0.82 eA-3

Alert level G

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension	3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF	?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.	5.30
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature	293 K
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	120
O3 -P1 -RB1 1.555 1.555 4.565	43.72 Deg.
PLAT793_ALERT_4_G The Model has Chirality at P1 (Verify)	R
PLAT793_ALERT_4_G The Model has Chirality at P2 (Verify)	S

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock shelxl - ellipsoid plot

